Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 74.8 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.56e-01

Confidence level: 6.92e-01

Nearest Neighbors from the Training Set

Image not found
Hexanal
Measured: 127
Predicted: 18.2

Image not found
Benzene, 1,2-difluoro-
Measured: 21.3
Predicted: 32.2

Image not found
Carbaryl
Measured: 59.3
Predicted: 1.44e-06

Image not found
Chloral
Measured: 71.3
Predicted: 41.1

Image not found
Camphor
Measured: 14.7
Predicted: 3.22e-01

Image not found
D-Camphor
Measured: 14.7
Predicted: 3.22e-01